Predicting ductility in quaternary *B2*-like alloys

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SUPPLEMENTARY MATERIAL

Table I contains calculated lattice parameters and elastic properties of the binary *B2* alloys with the PBE and PBEsol functionals while Table II contains the fault energies and metric quantities. For the 12 binary transition metal alloys, data from Sun and Johnson [S1] has been included for comparison. Table III contains calculated lattice parameters, elastic properties, and experimental hardnesses [S2] of the quaternary *B2*-like alloys while Table IV contains the fault energies and metric quantities.

The bulk modulus (B) and lattice parameter values were calculated by fitting to the Birch-Murnaghan equation of state while the isotropic shear modulus (c_{44}) was determined by applying volume-conserving monoclinic deformations to the unit cell and fitting to a known energy-volume relationship [S3], as described in the main text. Poisson's ratio (ν) was calculated using the relationship $G = c_{44}$ for isotropic cubic materials:

$$\nu = \frac{3B - 2G}{6B + 2G}$$

Although the only one of these quantities used directly in the metric is c_{44}, all calculated data is reported in the tables for completeness.

[S1] R. Sun and D. D. Johnson, Stability maps to predict anomalous ductility in B2 materials, Phys. Rev. B87, 104107 (2013).

[S2] P. L. Conway, B. Meyer, K. Scott, D. M. Miskovic, L. Bassman, and K. J. Laws, Ordering, strength and ductility in quaternary-to-octonary B2-structured transition-metal - rare-earth alloys, (Unpublished; for submission to Acta Mater.)

[S3] A. J. Zaddach, C. Niu, C. C. Koch, and D. L. Irving, Mechanical Properties and Stacking Fault Energies of NiFeCrCoMn High-Entropy Alloy, JOM 65, 1780-1789 (2013).

[S4] A. Dewaele, M. Torrent, P. Loubeyre, and M. Mezouar, "Compression Curves of Transition Metals in the Mbar Range: Experiments and Projector Augmented-Wave Calculations", Phys. Rev. B 78, 104102 (2008).

[S5] G. I. Csonka, J. P. Perdew, A. Ruzsinszky, P. H. T. Philipsen, S. Lebègue, J. Paier, O. A. Vydrov, and J. G. Ángyán, "Assessing the Performance of Recent Density Functionals for Bulk Solids", Phys. Rev. B 79, 155107 (2009).

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TABLE I. Binary *B2* alloy lattice parameter (a), bulk modulus (B), isotropic shear modulus (c_{44}), and Poisson's ratio (ν) calculated with the PBE and PBEsol functional approximations. Data from Sun and Johnson [S1] are listed on the second row of each of the transition metal alloys.

	PBE				PBEsol			
	a (Å)	B(GPa)	c_{44}(GPa)	ν	a (Å)	B (GPa)	c_{44} (GPa)	ν
AuZn[1]	3.187	95.834	44.977	0.297	3.229	31.290	30.667	0.131
	3.195	116.9	42.8	0.337				
FeAl	2.841	265.684	157.667	0.252	2.816	351.150	167.540	0.294
	2.879	161.3	130.2	0.182				
NiAl	2.863	171.835	128.206	0.201	2.831	204.102	140.159	0.221
	2.895	159.4	112.8	0.214				
ScAg	3.417	863.850	48.677	0.472	3.408	1054.491	47.577	0.478
	3.422	87.7	47.1	0.272				
ScAu	3.375	102.565	52.700	0.281	3.323	123.712	59.853	0.292
	3.393	111.9	47.4	0.314				
ScCu	3.231	112.299	55.083	0.289	3.192	149.253	58.909	0.326
	3.245	96.1	54.8	0.261				
ScPd	3.282	148.997	48.996	0.352	3.243	208.810	52.555	0.384
	3.301	119.9	42.8	0.341				
ScRu	3.181	176.007	51.675	0.366	3.145	221.407	59.680	0.376
	3.201	152.5	40.4	0.378				
YAg	3.647	72.738	33.804	0.299	3.590	77.938	37.367	0.293
	3.646	68.3	35	0.281				
YIn	3.756	60.900	45.448	0.201	3.701	75.045	51.332	0.221
	3.769	57.3	43.4	0.198				
YMg	3.791	41.132	41.799	0.120	3.747	44.222	44.851	0.121
	3.798	41.2	39.6	0.136				
YZn	3.565	61.032	44.772	0.205	3.506	72.603	50.234	0.219
	3.578	62.6	43.2	0.219				
AgLa	3.842	47.412	20.568	0.310	3.759	54.226	22.974	0.314
CuDy	3.457	76.823	38.652	0.285	3.398	97.562	42.663	0.309
CuGd	3.494	76.010	35.708	0.297	3.437	98.881	39.074	0.325
CuHo	3.776	60.870	14.581	0.389	3.738	64.450	15.056	0.392
MgCe	3.941	34.635	38.896	0.091	3.885	37.635	42.653	0.089
MgGd	3.803	40.176	41.187	0.118	3.751	43.961	44.611	0.121
MgHo	3.766	41.151	43.610	0.108	3.716	44.460	46.950	0.109
MgPr	3.907	35.997	35.523	0.129	3.852	39.302	39.941	0.120
ZnDy	3.555	58.654	45.845	0.190	3.487	69.341	51.282	0.203
ZnTb	3.572	57.020	44.203	0.192	3.502	67.114	48.656	0.208

[1] AuZn's unusual response to the change in functional approximation seems perhaps related to PBEsol's known overcorrection of Zn's properties and/or PBE's large errors compared to experiment [S4,S5].

TABLE II. Binary *B2* alloy APB$\{1\bar{1}0\}$, SF$\{1\bar{1}0\}$, and APB$\{11\bar{2}\}$ fault energies (reported in mJ/m^2) and dimensionless quantities λ, ln(C), and ln(δ) calculated with the PBE and PBEsol functional approximations. Results from Sun and Johnson [S1] are listed on the second row of each of the transition metal alloys.

	PBE						PBEsol					
	$\gamma_{\mathrm{APB}}^{1\bar{1}0}$	$\gamma_{\mathrm{SF}}^{1\bar{1}0}$	$\gamma_{\mathrm{APB}}^{11\bar{2}}$	λ	ln(C)	ln(δ)	$\gamma_{\mathrm{APB}}^{1\bar{1}0}$	$\gamma_{\mathrm{SF}}^{1\bar{1}0}$	$\gamma_{\mathrm{APB}}^{11\bar{2}}$	λ	ln(C)	ln(δ)
AuZn	213.524	491.179	252.762	1.184	-4.207	0.833	176.850	252.741	209.810	1.186	-4.025	0.357
	247	636	303	1.22	-4.262	0.948						
FeAl	348.731	1 831.244	693.917	1.990	-4.855	1.658	345.461	1975.803	712.415	2.062	-4.917	1.744
	348	1 248	403	1.16	-4.636	1.278						
NiAl	823.880	1 597.454	1 008.162	1.224	-3.797	0.662	888.288	1746.736	1084.470	1.221	-3.799	0.676
	777	1 379	971	1.25	-3.768	0.571						
ScAg	539.835	451.277	574.704	1.065	-3.428	-0.179	549.064	397.770	587.632	1.070	-3.385	-0.322
	548	437	598	1.25	-3.408	-0.227						
ScAu	791.900	334.450	866.354	1.094	-3.112	-0.862	826.947	383.475	918.695	1.111	-3.180	-0.768
	805	333	898	1.12	-3.088	-0.882						
ScCu	743.430	497.463	839.848	1.130	-3.176	-0.402	765.940	516.358	876.709	1.145	-3.201	-0.394
	713	406	830	1.16	-3.182	-0.564						
ScPd	817.534	293.509	883.497	1.081	-2.979	-1.024	849.896	308.993	917.732	1.080	-2.999	-1.012
	832	266	908	1.09	-2.888	-1.139						
ScRu	136.259	1 347.572	528.269	3.877	-4.793	2.292	112.541	1454.131	517.367	4.597	-5.117	2.559
	135	1 213	506	3.74	-4.556	2.194						
YAg	624.512	334.310	689.254	1.104	-2.983	-0.625	649.247	352.857	727.860	1.121	-3.028	-0.610
	641	364	732	1.14	-3.062	-0.564						
YIn	374.633	687.562	557.041	1.487	-3.819	0.607	425.204	797.071	611.031	1.437	-3.799	0.628
	757	322	931	1.23	-2.839	-0.856						
YMg	250.069	772.642	255.319	1.021	-4.149	1.128	306.484	816.941	254.992	0.832	-4.004	0.980
	277	714	259	0.93	-3.985	0.948						
YZn	579.701	592.241	685.689	1.183	-3.315	0.021	565.092	642.969	703.511	1.245	-3.439	0.129
	558	536	700	1.25	-3.324	-0.498						
AgLa	386.325	210.541	420.950	1.090	-3.018	-0.607	319.969	245.075	348.661	1.090	-3.296	-0.267
CuDy	764.522	369.921	904.477	1.183	-2.861	-0.726	774.356	391.010	912.478	1.178	-2.930	-0.683
CuGd	697.334	326.990	837.974	1.202	-2.884	-0.757	720.906	338.043	866.300	1.202	-2.925	-0.757
CuHo	262.625	13.495	484.056	1.843	-3.043	-2.968	193.868	-24.695	500.369	2.581	-3.368	-2.061
MgCe	198.429	677.742	274.909	1.385	-4.347	1.228	180.274	745.627	264.761	1.469	-4.521	1.420
MgGd	254.991	763.931	247.236	0.970	-4.118	1.097	244.201	833.489	247.316	1.013	-4.227	1.228
MgHo	268.860	792.357	210.437	0.783	-4.112	1.081	263.274	843.776	208.798	0.793	-4.194	1.165
MgPr	206.791	702.455	274.332	1.327	-4.207	1.223	189.059	771.728	266.204	1.408	-4.399	1.407
ZnDy	516.155	572.442	633.767	1.228	-3.452	0.104	491.867	646.230	650.978	1.323	-3.593	0.273
ZnTb	476.513	550.519	618.831	1.299	-3.501	0.144	454.456	637.772	637.508	1.403	-3.624	0.339

TABLE III. Quaternary *B2*-like alloy lattice parameter (a), bulk modulus (B), isotropic shear modulus (c_{44}), and Poisson's ratio (ν) calculated with the PBE and PBEsol functional approximations as well as experimental hardness values (± standard deviation) [S2]. Although the dimension of the quaternary *B2*-like unit cell shown in Fig. 1 of the main text is twice as long as the binary *B2* unit cell in any direction, the quaternary lattice parameters here are reported as the analog of the binary lattice parameters as a means of comparison.

	PBE				PBEsol				
	a (Å)	B(GPa)	c_{44}(GPa)	ν	a(Å)	B(GPa)	c_{44}(GPa)	ν	Experimental hardness (HV)
AgAuDyGd	7.262	75.436	33.563	0.306	7.147	80.673	36.588	0.303	159.4±5.4
AgAuDyY	7.230	73.227	35.143	0.293	7.128	81.048	37.921	0.298	166.6±13.5
AgAuGdY	7.267	75.150	33.455	0.306	7.161	79.827	36.234	0.303	159.9±11.4
AgAuScY	7.051	82.620	40.730	0.288	6.937	85.826	45.371	0.275	329.7±1.5
AgCuScY	6.947	72.790	39.935	0.268	6.834	79.261	44.263	0.265	383.3±9.1
AgPdDyGd	7.169	7.169	31.987	0.307	7.059	80.961	33.499	0.318	230.3±8.7
AgPdDyY	7.150	75.501	32.512	0.312	7.040	81.396	35.709	0.309	238.9±19.1
AgPdGdY	7.184	75.215	31.360	0.317	7.073	79.985	34.406	0.312	226.2±9.5
AgPdScY	6.965	82.299	36.731	0.306	6.857	86.331	40.763	0.296	402.7±15.0
AuPdScY	6.934	92.852	37.413	0.322	6.820	98.282	41.894	0.313	439.3±7.2
CuPdScY	6.810	86.827	37.405	0.312	6.690	90.450	42.329	0.298	369.0±15.7
AlHfNbTi	6.609	126.195	63.205	0.285	6.542	135.133	67.055	0.287	
AlHfTaTi	6.585	127.558	70.264	0.267	6.532	142.324	74.127	0.278	
AlMoNbTi	6.380	158.630	48.452	0.361	6.323	169.205	53.889	0.356	
AlNbTiV	6.342	147.747	64.905	0.308	6.285	155.885	67.051	0.312	

TABLE IV. Quaternary *B2*-like alloy APB$\{1\bar{1}0\}$, SF$\{1\bar{1}0\}$, and APB$\{11\bar{2}\}$ fault energies (reported in mJ/m^2) and dimensionless quantities λ, ln(C), and ln(δ) calculated with the PBE and PBEsol functional approximations.

	PBE						PBEsol					
	$\gamma_{\mathrm{APB}}^{1\bar{1}0}$	$\gamma_{\mathrm{SF}}^{1\bar{1}0}$	$\gamma_{\mathrm{APB}}^{11\bar{2}}$	λ	ln(C)	ln(δ)	$\gamma_{\mathrm{APB}}^{1\bar{1}0}$	$\gamma_{\mathrm{SF}}^{1\bar{1}0}$	$\gamma_{\mathrm{APB}}^{11\bar{2}}$	λ	ln(C)	ln(δ)
AgAuDyGd	927.038	860.668	802.551	0.866	−2.576	−0.074	745.630	284.900	837.941	1.124	−2.864	−0.962
AgAuDyY	763.506	298.561	836.643	1.096	−2.812	−0.939	775.703	288.344	867.647	1.119	−2.858	−0.990
AgAuGdY	736.544	278.502	810.978	1.101	−2.804	−0.973	748.219	274.195	838.384	1.121	−2.853	−1.004
AgAuScY	712.917	320.176	950.779	1.334	−3.003	−0.800	746.413	345.839	875.404	1.173	−3.048	−0.769
AgCuScY	672.273	358.002	752.034	1.119	−3.027	−0.630	688.504	379.410	798.919	1.160	−3.090	−0.596
AgPdDyGd	645.182	128.553	764.792	1.185	−2.878	−1.613	613.927	89.257	930.500	1.516	−2.958	−1.928
AgPdDyY	680.900	158.437	796.599	1.170	−2.837	−1.458	700.963	155.610	824.998	1.177	−2.887	−1.505
AgPdGdY	655.856	129.742	775.588	1.183	−2.843	−1.620	678.711	142.686	797.152	1.175	−2.886	−1.560
AgPdScY	662.135	244.482	743.871	1.123	−2.961	−0.996	686.272	245.133	827.760	1.206	−3.014	−1.029
AuPdScY	806.848	165.041	920.267	1.141	−2.777	−1.587	830.328	188.872	953.266	1.148	−2.845	−1.481
CuPdScY	847.736	248.111	865.238	1.021	−2.710	−1.229	767.648	277.195	897.874	1.170	−2.915	−1.019
AlHfNbTi	73.248	885.800	71.175	0.972	−5.653	2.493	80.248	948.834	73.436	0.915	−5.611	2.470
AlHfTaTi	15.148	962.701	21.716	1.434	−7.331	4.152	19.979	1 009.747	21.891	1.096	−7.100	3.923
AlMoNbTi	−543.453	625.976	−511.162	0.941	−3.348	0.141	−418.778	824.933	−532.416	1.271	−3.706	0.678
AlNbTiV	127.267	1 007.426	154.922	1.217	−5.086	2.069	120.032	1 042.873	139.039	1.158	−5.168	2.162